Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

Tetra-μ-acetato-*O*:*O*′-bis[(7-azaindole-*N*)copper(II)]

Yoshiyuki Kani, Masanobu Tsuchimoto and Shigeru Ohba*

Department of Chemistry, Faculty of Science and Technology, Keio University, Hiyoshi 3-14-1, Kohoku-ku, Yokohama 223-8522, Japan
Correspondence e-mail: ohba@chem.keio.ac.jp

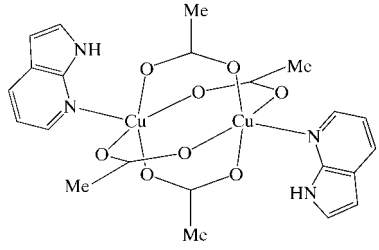
Received 31 March 2000
Accepted 11 April 2000

Data validation number: IUC0000104

The title complex, $[Cu_2(C_2H_3O_2)_4(C_7H_6N_2)_2]$, shows a binuclear cage structure having an inversion centre. There are intramolecular N—H···O hydrogen bonds between the 7-azaindole ligands and the bridging acetate O atoms.

Comment

The structure of the mixed-bridged binuclear copper(II) complex $[Cu_2(CH_3COO)_2(az)_2(Haz)_2]$ (Haz is 7-azaindole) was reported by Peng & Lai (1988). The structure of $[Cu_2(CH_3COO)_4(Haz)_2]$, (I), is reported here.



(I)

Experimental

1-Propanol (10 ml) solutions of copper(II) acetate monohydrate (0.5 mmol) and 7-azaindole (1 mmol) were mixed and filtered. From the light-blue–green filtrate, crystals of the title compound, $[Cu_2(CH_3COO)_4(Haz)_2]$, were obtained.

Crystal data

$[Cu_2(C_2H_3O_2)_4(C_7H_6N_2)_2]$
M_r = 599.55
Monoclinic, $P2_1/a$
a = 7.453 (5) Å
b = 14.911 (5) Å
c = 11.458 (5) Å
β = 107.75 (4)°
V = 1212.7 (10) Å^3
Z = 2
D_x = 1.642 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 10–15°
μ = 1.809 mm^{-1}
T = 298 K
Prism, green
0.2 × 0.1 × 0.1 mm

Data collection

Rigaku AFC-7*R* diffractometer
θ–2θ scans
Absorption correction: by integration (Coppens *et al.*, 1965)
T_{min} = 0.745, T_{max} = 0.854
3109 measured reflections
2779 independent reflections
1860 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 27.5°
$h = 0 \rightarrow 10$
$k = -19 \rightarrow 0$
$l = -15 \rightarrow 15$
3 standard reflections
every 150 reflections
intensity decay: none

Refinement

Refinement on F^2
$R(F)$ = 0.041
$wR(F^2)$ = 0.148
S = 0.93
2779 reflections
163 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + \{0.1(F_o^2 + 2F_c^2)/3\}^2]$
$(\Delta/\sigma)_{max}$ = 0.007
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—Cu1^{i}	2.651 (1)	Cu1—O3	1.975 (3)
Cu1—O1	1.974 (3)	Cu1—O4^{i}	1.997 (3)
Cu1—O2^{i}	1.976 (3)	Cu1—N1	2.177 (4)
O1—Cu1—O2^{i}	167.8 (1)	O1—C1—O2	125.6 (4)
O3—Cu1—O4^{i}	167.4 (1)	O3—C3—O4	124.5 (4)

Symmetry codes: (i) $2-x, -y, -z$.

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H1···O4^{i}	0.96	2.02	2.822 (6)	140

Symmetry code: (i) $2-x, -y, -z$.

The positional parameters of all the H atoms were calculated geometrically and fixed with U(H) = 1.2U_{eq}(parent atom).

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1993); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *TEXSAN*; software used to prepare material for publication: *TEXSAN*.

References

Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435–436.
Coppens, P., Leiserowitz, L. & Rabinovich, D. (1965). *Acta Cryst.* **18**, 1035–1038.
Molecular Structure Corporation (1993). *MSC/AFC Diffractometer Control Software*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
Molecular Structure Corporation (1999). *TEXSAN*. Version 1.10. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
Peng, S.-M. & Lai, C.-H. (1988). *J. Chin. Chem. Soc.* **35**, 325–336.